Parallel Molecular Docking

The front cover illustrates the parallel molecular docking of large databases on the Sequoia, a petascale IBM Blue Gene/Q supercomputer at Lawrence Livermore National Laboratory. A mixed parallel scheme that combines MPI and multithreading is implemented by Xiaohua Zhang, Sergio E. Wong, and Felice C. Lightstone on page 915 in the Vina molecular docking program named VinaLC, where LC stands for Livermore Computing. Parallel performance analysis shows the code scales up to more than 15K CPUs with a very low overhead cost of 3.94%. One million flexible compound docking calculations take only 1.4 hours on about 15K CPUs. The picture shows ligands that have been docked into various receptors to form ligand–receptor complexes via calculations on the Sequoia.

ATP Binding Site Prediction

TargetATPsite, a new method based on residue evolution image sparse representation and classifier ensemble, is developed for predicting ATP-binding sites from primary sequences, as presented by Dong-Jun Yu, Jun Hu, Yan Huang, Hong-Bin Shen, Yong Qi, Zhen-Min Tang, and Jing-Yu Yang on page 974. The high performance of TargetATPsite originates from the good discriminative capability of the new image sparse representation feature and the power of the modified AdaBoost classifier ensemble. TargetATPsite also features the capability of further identifying the binding pockets from the predicted binding residues through a spatial clustering algorithm.